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Russel Caflisch

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Mathematics Department
UCLA
Los Angeles, CA 90024

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FINAL REPORT

Nonlinear and Stochastic Numerical Methods and Their Applications

Grant #DAAL03-91-G-0162

Russel E. Caflisch, Principal Investigator

Mathematics Department UCLA
phone: 310-206-0200
fax: 310-206-6673
e-mail: caflisch@math.ucla.edu

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This grant was funded from July 1, 1991, through May 31, 1994. Research under the grant was concentrated on development of innovative numerical methods, in particular methods that are nonlinear and random, which are directly useful for computation in science and engineering. Our research also includes applications to problems in fluid mechanics, material science, transport theory and other fields. The results of this research are briefly described here, and the corresponding publications are listed at the end of the report.

1. Implicit Methods for Transport Theory

Numerical methods for transport processes become computationally expensive when the mean free path ε is small, i.e. in the diffusion (or fluid-dynamic) limit. Such problems occur in many applications, such as flight in the upper atmosphere, neutron transport in nuclear reactors, and design of semi-conductors, and present a fundamental challenge for numerical transport methods. In this limit the solution varies on a slow fluid-dynamic time scale that is much slower than the collisional time scale, and we wish to use a numerical method that only resolves the fluid-dynamic scale.

The goal of this project was to develop numerical methods that are robust and efficient for small ε, by requiring the $\varepsilon \to 0$ limit for the discretized transport equation to be a discretization of the limiting fluid or diffusion equations. In collaboration with Shi Jin (Georgia Tech) and Giovanni Russo (University of L'Aquila, Italy) Caflisch has developed a set of implicit finite difference methods for the Broadwell model of the Boltzmann equation. After careful choice of the method to insure consistency with the fluid-dynamic limit, the main remaining difficulty turns out to be one of stability, requiring use of implicit methods.

A fully implicit or linearly implicit finite difference method or a Strang splitting method with an implicit collision step have been used. These methods have been successful in simulating shock waves, even if the collisional time scale was not well resolved, using an upwind method that correctly captures the shock. Because of the implicit formulation, these methods are stable for any choice of mean free path ε and spatial discretization Δx. In particular in the fluid dynamic limit, the transport discretization converges to a discretization for the fluid dynamic equations. A mathematical analysis of this convergence and a computational demonstration of the accuracy of the method have been completed.

Finite difference methods are applicable to a limited set of transport problems. For the most difficult problems, such as rarefied gas dynamics in more than 1 space dimension, particle methods (most often Monte Carlo) are required. Finding particle methods with the same fluid dynamic behavior remains an open, challenging problem.

2. Multi-Phase Flow Multi-phase flows, such as flow of a liquid containing air bubbles, are complex phenomena requiring investigation on both the microscopic scale of a single bubble and the macroscopic scale of a mixture. We have collaborated on various problems in multi-phase flow, in particular bubbly liquids, using a spectrum of numerical and analytic methods, including the vortex sheet and dipole sheet formulations, the level set description, and a statistical theory for macroscopic behavior.

For a single bubble, we have considered the oscillations due to impulsive motion, gravitational force or an oscillating ambient pressure. The oscillations are asymmetric, and eventually one side of the bubble forms a jet which hits the other side and may break a hole in the bubble. This is a particularly challenging problem, which contains a number of unresolved physical, mathematical and numerical issues.

Caflisch, Pugh and Smereka have simulated this flow directly using the vortex sheet and vortex dipole methods, with an ad hoc reconnection at the time that the two sides nearly collide. We have then compared these results with numerical computations from the level set method (described below) applied to the bubble problem by Osher, Smereka and Sussman. The results show good agreement, which provides some validation of the three methods.

In a separate study, Pugh and his former advisor Stephen Cowley (Cambridge University) have performed an analysis of singularity formation on rising bubbles in the Boussinesq approximation. The bubble is unstable due to Rayleigh-Taylor instability, which generates vorticity on the interface. Then the interface is subject to Kelvin-Helmholtz instability, which produces a singularity in the curvature of the interface. They perform numerical computation for this problem, using a vortex method and a nonlinear filtering method that was first developed by Krasny. Then they analyze the spectrum of their numerical solution to detect the approach of singularities. Although their numerical method stops at this point, the interface is expected to role up after the appearance of the singularity. Part of this work was contained in Pugh's thesis at the University of London.

For a collection of bubbles in a liquid, Russo and Smereka have derived a Vlasov-Poisson equation for the evolution of the bubble distribution. With this formulation they are able to analyze the stability of different distributions and to predict bubble clumping for certain values of the macroscopic parameters. This theory gives an analytic explanation of the observed instability of a cloud of bubbles all moving at the same speed in an incompressible fluid.

3. Vortex Flows

We have investigated several problems for vortical flows, including generation of vorticity from viscous flow around an obstacle and generation of singularities in swirling, inviscid flow.

Anderson and a graduate student, Marc Reider, have performed a numerical study of viscous flow past a cylinder, including a boundary layer and its separation. Their simulations of the Prandtl equations show significant differences from the corresponding computations for the Navier Stokes equations. They did this for both finite difference methods and vortex methods. However, the Prandtl equations do lead to a simplification of the computational problem, and it was of interest to see if one could modify the methods which use the Prandtl equations so that the inaccuracy could be removed. As a result they have formulated an alternative to the Prandtl equations which eliminates the original inaccuracies. Their new approximation includes more coupling between the boundary layer flow and the external flow. This rather simple change improves the results dramatically. This work formed a part of Marc Reider's Ph.D. thesis.

Caflisch has performed an analysis and computation of axisymmetric flow with swirl in search of singularity formation for such flows. First the equations are approximated using Moore's approximation, which keeps nonlinear interactions that send energy to higher wavenumbers, but omits those that send energy back to lower wavenumbers. This is expected to be a good approximation for singularity formation, and in particular it has been shown to give excellent results for singularity formation in interface problems. The result of this approximation is to split the Euler solution into two parts: the upper analytic part of the velocity and the lower analytic part, each of which is complex and solves the original Euler equations. Special traveling wave solutions are then constructed numerically for these complex Euler equations, and singularities are found to form at a finite real time. The connection of these solutions with real Euler solutions is now being investigated.

4. The Level Set Approach to Interfacial Dynamics

In an earlier investigation, Stanley Osher and Barry Merriman discovered a new algorithm for moving a curve by mean curvature. In this new method, the curve is moved by a simple algorithm involving diffusion of a set bounded by the curve at each time step. By a straightforward modification this method can also be formulated for triple points, which has been a major stumbling block for other algorithms, such as the Osher-Sethian method. An analysis of this algorithm has been completed by Pierre Mascarenhas, who was a long term visitor at UCLA from Ecole Polytechnique in France. He has established the convergence of the algorithm for both regular curves and curves with triple points. He has also run a number of test cases to document the accuracy and efficiency of the method. This method is expected to have a major impact on problems, such as crystal growth, that involve motion by mean curvature. The method has also been successfully extended to 3D.

This same approach, representing the interface as the level set of a function, has been implemented to describe the dynamics of a bubble interface. In this case, the interface velocity is determined by solving an elliptic problem in the domain.

5. Quasi-Monte Carlo Methods

Monte Carlo methods are one of the most commonly used numerical methods for simulation and integration but have received little attention from the applied mathematics and numerical analysis communities. Even small progress in improving these methods can result in a large payoff. We have tried to bring the methods of applied math, including controlled computational experiments and a geometric point of view to these methods. In particular we have investigated the effectiveness of quasi-random methods, which are a deterministic alternative to the usual random (or pseudo random, which attempts to simulate random) methods.

In earlier work, we showed that the effectiveness of quasi-random methods is greatly reduced for problems in high dimension or in which the integrand is not smooth. To remedy this situation, Caflisch and Moskowitz developed modified Monte Carlo methods in which the integrand is smoothed or the effective dimension is reduced. The methods include the acceptance-rejection method, Feynman-Kac integration and Diffusion Monte Carlo, all of which were modified to make them smooth and to reduce the effective dimension. Moskowitz has further developed this approach and applied it to some significant problems, such as the ground state of the hydrogen and helium atoms.

6. Shock Capturing Methods

Osher and his student X. Liu have been working on simplifications and theoretical improvements of essentially nonoscillatory (ENO) approximations for hyperbolic conservation laws. They have two main results:

Instead of using an adaptive stencil based on "left" or "right" choice at each level of accuracy, they use a nonlinear weighting of the Newton coefficients, i.e. increasing functions of smoothness. This approach is inherently multi-dimensional. Preliminary multidimensional results are very encouraging.

They have devised a central difference based third order accurate non-oscillatory method for which a maximum principle (in the scalar case) can be proven. This method is as nonoscillatory as basic third order ENO but is more accurate (lower truncation error) in practice, and provides some hope of yielding a convergence theory.

Shock capturing methods were used for the computation of inviscid detonation waves. Due to the speed of the chemical reactions, previous capturing methods gave a significant over-estimate of the speed of the combustion wave. The new methods were shown to overcome this difficulty.

Personnel Supported under this Grant

Faculty
Christopher Anderson
Russel Caflisch
Bjorn Engquist
Stanley Osher

Postdocs
David Pugh
Peter Smereka

Publications from Research Supported This Grant

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